



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2022 – 02:10 pm BST

PDB ID : 7Q69
Title : Crystal structure of Chaetomium thermophilum C30S Ahp1 in the pre-reaction state
Authors : Ravichandran, K.E.; Wilk, P.; Grudnik, P.; Glatt, S.
Deposited on : 2021-11-05
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

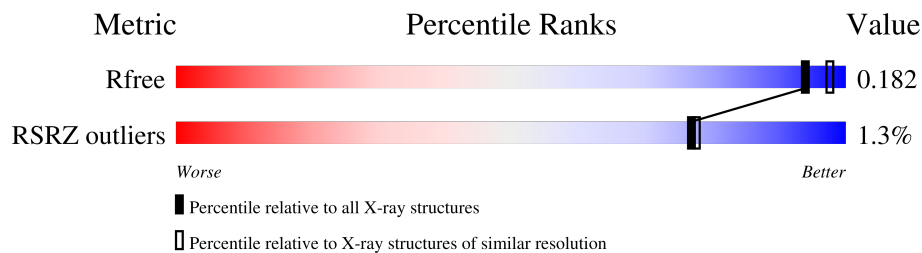
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---------------|-----------------------------|---|
| R_{free} | 130704 | 2469 (1.86-1.86) |
| RSRZ outliers | 127900 | 2436 (1.86-1.86) |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11035 atoms, of which 5032 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thioredoxin domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | H | N | O | S | | | |
| 1 | A | 174 | 2581 | 816 | 1291 | 218 | 253 | 3 | 10 | 5 | 0 |
| 1 | B | 169 | 2528 | 802 | 1259 | 214 | 250 | 3 | 0 | 3 | 0 |
| 1 | C | 167 | 2475 | 786 | 1234 | 210 | 243 | 2 | 13 | 1 | 0 |
| 1 | D | 166 | 2471 | 785 | 1233 | 209 | 242 | 2 | 20 | 3 | 0 |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | -1 | GLY | - | expression tag | UNP G0S1P8 |
| A | 0 | ALA | - | expression tag | UNP G0S1P8 |
| A | 30 | SER | CYS | engineered mutation | UNP G0S1P8 |
| B | -1 | GLY | - | expression tag | UNP G0S1P8 |
| B | 0 | ALA | - | expression tag | UNP G0S1P8 |
| B | 30 | SER | CYS | engineered mutation | UNP G0S1P8 |
| C | -1 | GLY | - | expression tag | UNP G0S1P8 |
| C | 0 | ALA | - | expression tag | UNP G0S1P8 |
| C | 30 | SER | CYS | engineered mutation | UNP G0S1P8 |
| D | -1 | GLY | - | expression tag | UNP G0S1P8 |
| D | 0 | ALA | - | expression tag | UNP G0S1P8 |
| D | 30 | SER | CYS | engineered mutation | UNP G0S1P8 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2 | A | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | A | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | A | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | B | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | B | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | B | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | C | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | C | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | C | 1 | Total O S 5 4 1 | 0 | 0 |
| 2 | D | 1 | Total O S 5 4 1 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| | | | Total | C | H | O | | |
| 3 | B | 1 | 11 | 3 | 5 | 3 | 0 | 0 |
| 3 | C | 1 | 11 | 3 | 5 | 3 | 0 | 0 |
| 3 | D | 1 | 11 | 3 | 5 | 3 | 0 | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| | | | Total | O | | |
| 4 | A | 250 | 250 | 250 | 0 | 0 |
| 4 | B | 241 | 241 | 241 | 0 | 0 |
| 4 | C | 253 | 253 | 253 | 0 | 0 |
| 4 | D | 153 | 153 | 153 | 0 | 0 |

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3 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 60.14Å 101.73Å 69.42Å 90.00° 107.33° 90.00° | Depositor |
| Resolution (Å) | 46.07 – 1.85 46.07 – 1.85 | Depositor EDS |
| % Data completeness (in resolution range) | 96.1 (46.07-1.85) 96.2 (46.07-1.85) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.01 (at 1.84Å) | Xtriage |
| Refinement program | PHENIX 1.18.2-3874 | Depositor |
| R, R_{free} | 0.157 , 0.183 0.156 , 0.182 | Depositor DCC |
| R_{free} test set | 3284 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 18.9 | Xtriage |
| Anisotropy | 0.091 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | (Not available) , (Not available) | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 11035 | wwPDB-VP |
| Average B, all atoms (Å ²) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | B | 204 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.05 | 0 |
| 3 | GOL | B | 201 | - | 5,5,5 | 0.99 | 1 (20%) | 5,5,5 | 0.88 | 0 |
| 3 | GOL | C | 201 | - | 5,5,5 | 1.06 | 1 (20%) | 5,5,5 | 1.04 | 0 |
| 2 | SO4 | A | 201 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.11 | 0 |
| 2 | SO4 | B | 202 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | C | 203 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.16 | 0 |
| 2 | SO4 | C | 204 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.09 | 0 |
| 3 | GOL | D | 201 | - | 5,5,5 | 0.63 | 0 | 5,5,5 | 1.03 | 0 |
| 2 | SO4 | A | 203 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.10 | 0 |
| 2 | SO4 | A | 202 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | C | 202 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 203 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.11 | 0 |
| 2 | SO4 | D | 202 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | GOL | C | 201 | - | - | 2/4/4/4 | - |
| 3 | GOL | D | 201 | - | - | 4/4/4/4 | - |
| 3 | GOL | B | 201 | - | - | 2/4/4/4 | - |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | B | 201 | GOL | O2-C2 | -2.13 | 1.37 | 1.43 |
| 3 | C | 201 | GOL | O2-C2 | -2.00 | 1.37 | 1.43 |

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | B | 201 | GOL | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | C | 201 | GOL | O1-C1-C2-C3 |
| 3 | D | 201 | GOL | O1-C1-C2-C3 |
| 3 | D | 201 | GOL | C1-C2-C3-O3 |
| 3 | D | 201 | GOL | O2-C2-C3-O3 |

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|------------------------------|-----------------------|--------|
| 1 | A | 174/174 (100%) | -0.41 | 0 100 100 | 12, 19, 38, 68 | 1 (0%) |
| 1 | B | 169/174 (97%) | -0.43 | 2 (1%) 79 79 | 11, 17, 31, 53 | 0 |
| 1 | C | 167/174 (95%) | -0.44 | 1 (0%) 89 89 | 13, 20, 35, 55 | 1 (0%) |
| 1 | D | 166/174 (95%) | 0.01 | 6 (3%) 42 40 | 16, 34, 54, 72 | 3 (1%) |
| All | All | 676/696 (97%) | -0.32 | 9 (1%) 77 78 | 11, 21, 46, 72 | 5 (0%) |

The worst 5 of 9 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 1 | B | 1 | MET | 3.1 |
| 1 | D | 72 | LEU | 2.9 |
| 1 | D | 76 | ARG | 2.6 |
| 1 | D | 70 | ALA | 2.5 |
| 1 | D | 77[A] | GLN | 2.4 |

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | GOL | B | 201 | 6/6 | 0.88 | 0.19 | 27,34,46,46 | 0 |
| 3 | GOL | D | 201 | 6/6 | 0.88 | 0.25 | 50,57,80,96 | 0 |
| 2 | SO4 | B | 204 | 5/5 | 0.90 | 0.18 | 57,66,82,84 | 0 |
| 2 | SO4 | C | 204 | 5/5 | 0.92 | 0.19 | 47,50,61,63 | 5 |
| 2 | SO4 | B | 203 | 5/5 | 0.92 | 0.11 | 38,41,52,53 | 5 |
| 2 | SO4 | A | 202 | 5/5 | 0.92 | 0.15 | 34,43,55,59 | 5 |
| 3 | GOL | C | 201 | 6/6 | 0.93 | 0.14 | 31,42,51,51 | 0 |
| 2 | SO4 | A | 203 | 5/5 | 0.93 | 0.20 | 40,44,63,66 | 0 |
| 2 | SO4 | D | 202 | 5/5 | 0.95 | 0.09 | 49,50,58,59 | 5 |
| 2 | SO4 | C | 202 | 5/5 | 0.95 | 0.17 | 35,36,41,42 | 5 |
| 2 | SO4 | C | 203 | 5/5 | 0.96 | 0.09 | 31,34,40,40 | 5 |
| 2 | SO4 | A | 201 | 5/5 | 0.97 | 0.10 | 33,36,41,42 | 5 |
| 2 | SO4 | B | 202 | 5/5 | 0.98 | 0.09 | 28,31,37,40 | 5 |

5.5 Other polymers [i](#)

There are no such residues in this entry.